

Bis(2-methoxybenzylammonium) diaqua-bis(dihydrogen diphosphato- κ^2O,O' -cobaltate(II) dihydrateAdel Elbouali,^a Ahmed Selmi,^{a*} Nicolas Ratel-Ramond,^b Mohamed Rzaigui^a and Samah Toumi Akriche^a^aLaboratoire de Chimie des Matériaux, Faculté des Sciences de Bizerte, 7021 Zarzouna Bizerte, Tunisia, and ^bCEMES-CNRS, 29 rue Jeanne Marvig, 31055 Toulouse cedex 4, France
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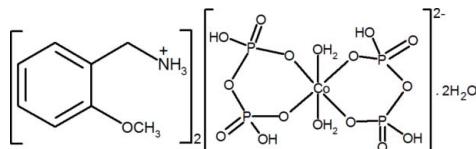
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Key indicators: single-crystal X-ray study; $T = 293\text{ K}$; mean $\sigma(\text{C}-\text{C}) = 0.014\text{ \AA}$; R factor = 0.096; wR factor = 0.266; data-to-parameter ratio = 21.9.

The title compound, $(\text{C}_8\text{H}_{12}\text{NO})_2[\text{Co}(\text{H}_2\text{P}_2\text{O}_7)_2(\text{H}_2\text{O})_2] \cdot 2\text{H}_2\text{O}$, crystallizes isotropically with its Mn^{II} analogue. It consists of alternating layers of organic cations and inorganic complex anions, extending parallel to (100). The complex cobaltate(II) anion exhibits $\overline{1}$ symmetry. Its Co^{2+} atom has an octahedral coordination sphere, defined by two water molecules in apical positions and two $\text{H}_2\text{P}_2\text{O}_7^{2-}$ ligands in equatorial positions. The cohesion between inorganic and organic layers is accomplished by a set of $\text{O}-\text{H}\cdots\text{O}$ and $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds involving the organic cation, the inorganic anion and the remaining lattice water molecules.

Related literature

For the isotropic Mn^{II} structure, see: Elbouali *et al.* (2013b). For related structures with diphosphate units, see: Alaoui Tahiri *et al.* (2003); Essehli *et al.* (2005); Selmi *et al.* (2006, 2009); Ahmed *et al.* (2006); Gharbi *et al.* (1994); Gharbi & Jouini (2004); Elbouali *et al.* (2013a). For distortion index calculations, see: Kobashi *et al.* (1997).

**Experimental***Crystal data*

$(\text{C}_8\text{H}_{12}\text{NO})_2[\text{Co}(\text{H}_2\text{P}_2\text{O}_7)_2(\text{H}_2\text{O})_2] \cdot 2\text{H}_2\text{O}$	$b = 11.971(5)\text{ \AA}$
	$c = 9.161(5)\text{ \AA}$
	$\beta = 93.718(5)^\circ$
	$V = 1537.6(12)\text{ \AA}^3$
	$Z = 2$

Mo $K\alpha$ radiation
 $\mu = 0.85\text{ mm}^{-1}$ $T = 293\text{ K}$
 $0.25 \times 0.19 \times 0.13\text{ mm}$ *Data collection*Nonius KappaCCD diffractometer
33422 measured reflections
4645 independent reflections3135 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.081$ *Refinement* $R[F^2 > 2\sigma(F^2)] = 0.096$
 $wR(F^2) = 0.266$
 $S = 1.08$
4645 reflections
212 parameters
7 restraintsH atoms treated by a mixture of
independent and constrained
refinement
 $\Delta\rho_{\text{max}} = 2.59\text{ e \AA}^{-3}$
 $\Delta\rho_{\text{min}} = -1.26\text{ e \AA}^{-3}$ **Table 1**
Selected bond lengths (\AA).

Co1–O1	2.075 (4)	Co1–O5	2.124 (4)
Co1–O1W	2.095 (4)		

Table 2
Hydrogen-bond geometry (\AA , $^\circ$).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
O3–H3 \cdots O2 ⁱ	0.82	1.85	2.553 (6)	143
O6–H6 \cdots O7 ⁱⁱ	0.82	1.77	2.571 (6)	166
O1W–H1W1 \cdots O2 ⁱⁱⁱ	0.86 (2)	1.98 (3)	2.827 (6)	168 (7)
O1W–H2W1 \cdots O7 ⁱⁱ	0.86 (2)	2.00 (2)	2.851 (6)	171 (8)
N1–H1A \cdots O2W	0.89	1.99	2.840 (8)	159
N1–H1A \cdots O3 ⁱⁱ	0.89	2.53	2.988 (7)	113
N1–H1B \cdots O5 ^{iv}	0.89	2.04	2.810 (7)	145
N1–H1C \cdots O1	0.89	2.28	2.944 (7)	131
N1–H1C \cdots O8	0.89	2.42	2.972 (9)	120
O2W–H1W2 \cdots O2 ⁱⁱ	0.85 (2)	2.08 (4)	2.885 (7)	157 (9)
O2W–H2W2 \cdots O7 ⁱⁱⁱ	0.85 (2)	2.06 (4)	2.876 (7)	161 (9)

Symmetry codes: (i) $x, -y + \frac{1}{2}, z + \frac{1}{2}$; (ii) $x, -y + \frac{1}{2}, z - \frac{1}{2}$; (iii) $-x + 1, y + \frac{1}{2}, -z + \frac{1}{2}$; (iv) $-x + 1, -y + 1, -z + 1$.

Data collection: *COLLECT* (Hooft, 1998); cell refinement: *DIRAX/LSQ* (Duisenberg *et al.*, 2000); data reduction: *EVALCCD* (Duisenberg *et al.*, 2003); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012) and *DIAMOND* (Brandenburg & Putz, 2005); software used to prepare material for publication: *WinGX* (Farrugia, 2012).

Supporting information for this paper is available from the IUCr electronic archives (Reference: WM5011).

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supplementary materials

Acta Cryst. (2014). E70, m145–m146 [doi:10.1107/S1600536814006102]

Bis(2-methoxybenzylammonium) diaquabis(dihydrogen diphosphato- κ^2O,O')cobaltate(II) dihydrate

Adel Elbouali, Ahmed Selmi, Nicolas Ratel-Ramond, Mohamed Rzaigui and Samah Toumi Akriche

1. Comment

As a part of our interest in diphosphate materials, we report here the preparation and the structural study of the title compound, $(C_8H_{12}NO)_2[Co(H_2P_2O_7)_2(H_2O)_2] \cdot 2H_2O$, (I), that crystallizes isotropically with its Mn^{II} analogue (Elbouali *et al.*, 2013*b*).

The asymmetric unit of (I) consists of a Co(II) atom, one $H_2P_2O_7^{2-}$ anion, one organic cation and two water molecules (one coordinating to Co(II) and the other a lattice water molecule). The Co(II) ion lies on an inversion centre, hence the complete formula unit is generated by this element of symmetry (Fig. 1).

The crystal structure of (I) exhibits the same type of architecture than that of the isotropic Mn^{II} analogue. It is built up from centrosymmetric $[Co(H_2P_2O_7)_2(H_2O)_2]^{2-}$ complex anions arranged in layers parallel to (100). These layers are interconnected by a set of O—H···O and N—H···O hydrogen bonds (Table 2, Fig. 2) between the components.

The distortion index calculation (Kobashi *et al.*, 1997) of the CoO_6 octahedron in the anion gives a value of 0.023, indicating a rather regular coordination sphere for this ion (radius 0.74 Å). The distortion index for the MnO_6 octahedron in the isotropic Mn^{II} analogue is with 0.028 slightly greater, probably as a consequence of the larger ionic radius of Mn^{II} (0.80 Å). The Co—O bond lengths around Co^{2+} ion are between 2.075 (4) and 2.124 (4) Å (Table 1), similar to those observed in $(NH_4)_2[Co(H_2P_2O_7)_2(H_2O)_2]$ (Essehli *et al.*, 2005) and due to the smaller ionic radius shorter than in $[Mn(H_2P_2O_7)_2(H_2O)_2]$ units in related structures (Alaoui Tahiri *et al.*, 2003; Elbouali *et al.*, 2013*b*).

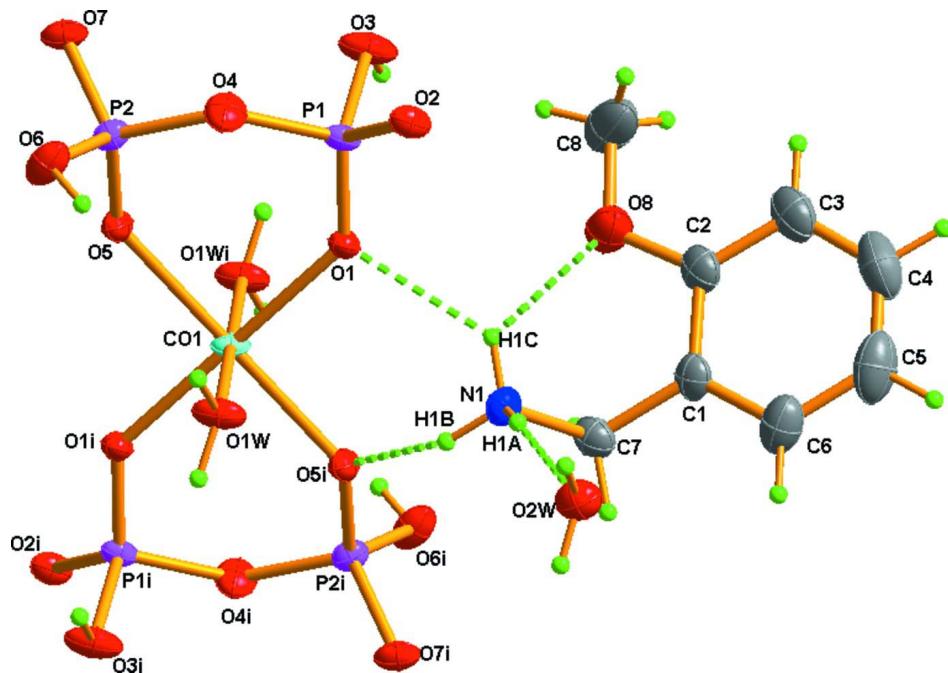
The P_2O_7 moiety has a quasi-eclipsed conformation with a mean O—P—O—P torsion angle of 19.6 ° and bridges the Co(II) ion through O1—P1 and O5—P2 linkages. The P_2O_7 group is bent, with a P1—O4—P2 bond angle of 132.9 (3)° as observed in other $M(II)$ –organic diphosphate frameworks (Elbouali *et al.* 2013*a*; Selmi *et al.* 2006, 2009; Ahmed *et al.* 2006; Gharbi *et al.* 2004, 1994).

2. Experimental

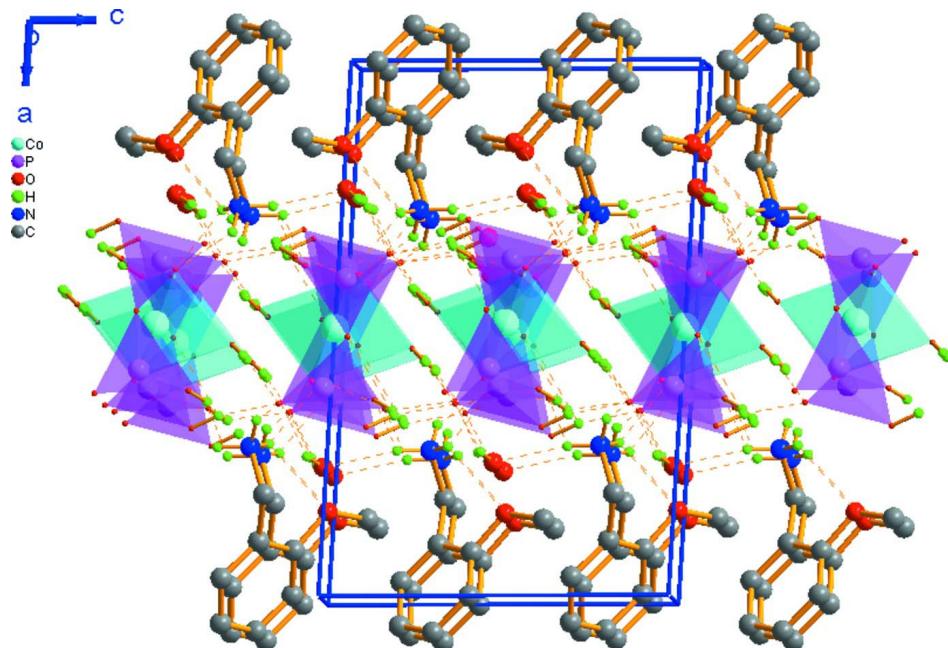
Crystals of the title compound were obtained by the reaction of diphosphoric acid (2 mmol), $CoCl_2 \cdot 6H_2O$ (0.24 g; 1 mmol) and 2-methoxybenzylamine (0.138 g; 1 mmol) carried out in an acidic medium. Diphosphoric acid, $H_4P_2O_7$, was obtained from $Na_4P_2O_7$ by using an ion-exchange resin (Amberlite IR 120).

3. Refinement

All H atoms attached to C, O and N atoms were fixed geometrically and treated as riding, with C—H = 0.93 Å with $U_{iso}(H) = 1.2U_{eq}(C)$ for aromatic ring and C—H = 0.97 and 0.96 Å and N—H = 0.89 Å, respectively, for CH_2 , CH_3 and NH_3 units and O—H = 0.82 Å for the hydrogen diphosphate anion with $U_{iso}(H) = 1.5U_{eq}(C, O \text{ or } N)$. The water H atoms were refined using restraints [O—H = 0.85 (1) Å, H···H = 1.44 (2) Å ° and $U_{iso}(H) = 1.5U_{eq}(O)$].

**Figure 1**

The molecular entities in the structure of (I) with the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are represented as small spheres of arbitrary radius. Hydrogen bonds are represented as dashed lines. [Symmetry code: (i) $1 - x, 1 - y, 1 - z$.]

**Figure 2**

Perspective view of the crystal packing of (I) in a projection along [010]. The H-atoms not involved in hydrogen bonding were omitted.

Bis(2-methoxybenzylammonium) diaquabis(dihydrogen diphosphato- κ^2O,O')cobaltate(II) dihydrate*Crystal data*

$M_r = 759.28$

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 14.050 (5)$ Å

$b = 11.971 (5)$ Å

$c = 9.161 (5)$ Å

$\beta = 93.718 (5)^\circ$

$V = 1537.6 (12)$ Å³

$Z = 2$

$F(000) = 786$

$D_x = 1.640$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 33422 reflections

$\theta = 2.2\text{--}30.9^\circ$

$\mu = 0.85$ mm⁻¹

$T = 293$ K

Prism, pink

$0.25 \times 0.19 \times 0.13$ mm

Data collection

Nonius KappaCCD

diffractometer

Radiation source: fine-focus sealed tube

Horizontally mounted graphite crystal
monochromator

Detector resolution: 9 pixels mm⁻¹

ω and φ CCD rotation images, thick slices scans
33422 measured reflections

4645 independent reflections

3135 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.081$

$\theta_{\text{max}} = 30.9^\circ$, $\theta_{\text{min}} = 2.2^\circ$

$h = -20 \rightarrow 18$

$k = -17 \rightarrow 17$

$l = -10 \rightarrow 13$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.096$

$wR(F^2) = 0.266$

$S = 1.08$

4645 reflections

212 parameters

7 restraints

Primary atom site location: structure-invariant
direct methods

Secondary atom site location: difference Fourier
map

Hydrogen site location: inferred from
neighbouring sites

H atoms treated by a mixture of independent
and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0687P)^2 + 17.5972P]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\text{max}} = 0.003$

$\Delta\rho_{\text{max}} = 2.59$ e Å⁻³

$\Delta\rho_{\text{min}} = -1.26$ e Å⁻³

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) etc. and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^* / U_{\text{eq}}$
Co1	0.5000	0.5000	0.5000	0.0248 (3)
P1	0.58873 (11)	0.24678 (12)	0.46988 (14)	0.0240 (3)
P2	0.38517 (11)	0.25622 (12)	0.51633 (14)	0.0249 (3)
O1	0.5946 (3)	0.3708 (3)	0.4662 (4)	0.0278 (8)

O2	0.6336 (3)	0.1843 (3)	0.3488 (4)	0.0302 (9)
O3	0.6288 (4)	0.1972 (4)	0.6168 (5)	0.0471 (13)
H3	0.6494	0.2477	0.6704	0.071*
O4	0.4796 (4)	0.2083 (4)	0.4534 (6)	0.0446 (12)
O5	0.3993 (3)	0.3764 (4)	0.5528 (5)	0.0309 (9)
O6	0.3105 (4)	0.2386 (5)	0.3853 (5)	0.0434 (12)
H6	0.3333	0.2586	0.3094	0.065*
O7	0.3549 (4)	0.1825 (4)	0.6378 (4)	0.0349 (10)
O1W	0.4616 (4)	0.4955 (4)	0.2753 (5)	0.0402 (11)
H1W1	0.441 (6)	0.558 (3)	0.240 (8)	0.060*
H2W1	0.435 (5)	0.438 (3)	0.233 (8)	0.060*
O8	0.8402 (5)	0.3749 (6)	0.5079 (7)	0.0663 (18)
N1	0.7205 (4)	0.4951 (5)	0.2793 (6)	0.0369 (12)
H1A	0.7210	0.4784	0.1847	0.055*
H1B	0.6716	0.5403	0.2934	0.055*
H1C	0.7145	0.4327	0.3307	0.055*
C1	0.8971 (5)	0.4798 (7)	0.3192 (8)	0.0454 (17)
C2	0.9128 (6)	0.3901 (7)	0.4183 (9)	0.0514 (19)
C3	0.9953 (7)	0.3286 (9)	0.4206 (12)	0.068 (3)
H3A	1.0057	0.2708	0.4875	0.082*
C4	1.0628 (8)	0.3536 (11)	0.3228 (15)	0.085 (4)
H4	1.1191	0.3126	0.3253	0.101*
C5	1.0490 (8)	0.4362 (13)	0.2235 (14)	0.087 (4)
H5	1.0952	0.4509	0.1578	0.105*
C6	0.9657 (7)	0.4997 (10)	0.2192 (11)	0.071 (3)
H6A	0.9559	0.5555	0.1493	0.085*
C7	0.8106 (5)	0.5514 (7)	0.3277 (9)	0.0474 (17)
H7A	0.8066	0.5760	0.4280	0.057*
H7B	0.8179	0.6173	0.2679	0.057*
C8	0.8535 (9)	0.2951 (13)	0.6208 (15)	0.103 (5)
H8A	0.8584	0.2220	0.5788	0.154*
H8B	0.8003	0.2973	0.6812	0.154*
H8C	0.9110	0.3118	0.6791	0.154*
O2W	0.7511 (4)	0.4927 (5)	-0.0240 (6)	0.0487 (13)
H1W2	0.732 (6)	0.435 (4)	-0.071 (9)	0.073*
H2W2	0.732 (7)	0.555 (3)	-0.061 (9)	0.073*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.0412 (6)	0.0166 (5)	0.0165 (4)	0.0007 (4)	0.0011 (4)	0.0000 (4)
P1	0.0361 (8)	0.0222 (7)	0.0139 (5)	0.0062 (5)	0.0016 (5)	0.0004 (5)
P2	0.0336 (7)	0.0266 (7)	0.0144 (6)	-0.0044 (6)	0.0011 (5)	-0.0018 (5)
O1	0.031 (2)	0.0224 (19)	0.030 (2)	0.0035 (15)	0.0028 (16)	0.0026 (15)
O2	0.047 (3)	0.029 (2)	0.0150 (16)	0.0088 (17)	0.0041 (16)	-0.0026 (14)
O3	0.089 (4)	0.034 (3)	0.0170 (19)	0.015 (3)	-0.004 (2)	0.0004 (17)
O4	0.050 (3)	0.026 (2)	0.059 (3)	-0.002 (2)	0.009 (2)	-0.018 (2)
O5	0.032 (2)	0.028 (2)	0.034 (2)	0.0022 (16)	0.0104 (17)	-0.0002 (16)
O6	0.047 (3)	0.066 (3)	0.0172 (18)	-0.019 (2)	-0.0035 (18)	0.005 (2)
O7	0.057 (3)	0.029 (2)	0.0189 (18)	-0.0036 (19)	0.0000 (18)	0.0025 (15)

O1W	0.072 (3)	0.026 (2)	0.0205 (19)	0.002 (2)	-0.014 (2)	-0.0017 (16)
O8	0.058 (4)	0.087 (5)	0.052 (3)	-0.003 (3)	-0.001 (3)	0.022 (3)
N1	0.039 (3)	0.040 (3)	0.032 (3)	-0.001 (2)	0.006 (2)	-0.003 (2)
C1	0.035 (4)	0.059 (5)	0.041 (4)	-0.004 (3)	-0.006 (3)	-0.004 (3)
C2	0.039 (4)	0.058 (5)	0.054 (5)	-0.003 (3)	-0.012 (3)	-0.005 (4)
C3	0.051 (5)	0.073 (7)	0.078 (7)	0.003 (4)	-0.021 (5)	-0.013 (5)
C4	0.053 (6)	0.099 (9)	0.100 (9)	0.018 (6)	-0.006 (6)	-0.037 (8)
C5	0.062 (7)	0.130 (11)	0.072 (7)	-0.013 (7)	0.022 (5)	-0.036 (7)
C6	0.055 (6)	0.102 (8)	0.055 (5)	-0.016 (5)	0.007 (4)	-0.002 (5)
C7	0.047 (4)	0.046 (4)	0.048 (4)	0.002 (3)	-0.007 (3)	-0.002 (3)
C8	0.069 (7)	0.140 (12)	0.096 (9)	-0.025 (7)	-0.019 (6)	0.058 (9)
O2W	0.056 (3)	0.051 (3)	0.038 (3)	-0.005 (3)	-0.003 (2)	0.001 (2)

Geometric parameters (\AA , $\text{^{\circ}}$)

Co1—O1 ⁱ	2.075 (4)	N1—H1A	0.8900
Co1—O1	2.075 (4)	N1—H1B	0.8900
Co1—O1W ⁱ	2.095 (4)	N1—H1C	0.8900
Co1—O1W	2.095 (4)	C1—C6	1.393 (12)
Co1—O5	2.124 (4)	C1—C2	1.414 (12)
Co1—O5 ⁱ	2.124 (4)	C1—C7	1.494 (11)
P1—O1	1.488 (4)	C2—C3	1.373 (12)
P1—O2	1.509 (4)	C3—C4	1.379 (17)
P1—O3	1.543 (4)	C3—H3A	0.9300
P1—O4	1.598 (5)	C4—C5	1.349 (18)
P2—O5	1.488 (5)	C4—H4	0.9300
P2—O7	1.503 (4)	C5—C6	1.393 (16)
P2—O6	1.556 (4)	C5—H5	0.9300
P2—O4	1.588 (5)	C6—H6A	0.9300
O3—H3	0.8200	C7—H7A	0.9700
O6—H6	0.8200	C7—H7B	0.9700
O1W—H1W1	0.86 (2)	C8—H8A	0.9600
O1W—H2W1	0.86 (2)	C8—H8B	0.9600
O8—C2	1.362 (11)	C8—H8C	0.9600
O8—C8	1.411 (12)	O2W—H1W2	0.85 (2)
N1—C7	1.477 (9)	O2W—H2W2	0.85 (2)
O1 ⁱ —Co1—O1	180.0 (2)	C7—N1—H1B	109.5
O1 ⁱ —Co1—O1W ⁱ	87.73 (18)	H1A—N1—H1B	109.5
O1—Co1—O1W ⁱ	92.27 (18)	C7—N1—H1C	109.5
O1 ⁱ —Co1—O1W	92.27 (18)	H1A—N1—H1C	109.5
O1—Co1—O1W	87.73 (18)	H1B—N1—H1C	109.5
O1W ⁱ —Co1—O1W	180.000 (1)	C6—C1—C2	117.8 (8)
O1 ⁱ —Co1—O5	92.42 (16)	C6—C1—C7	122.5 (8)
O1—Co1—O5	87.58 (16)	C2—C1—C7	119.7 (7)
O1W ⁱ —Co1—O5	85.82 (19)	O8—C2—C3	125.7 (9)
O1W—Co1—O5	94.18 (19)	O8—C2—C1	113.4 (7)
O1 ⁱ —Co1—O5 ⁱ	87.58 (16)	C3—C2—C1	120.9 (9)
O1—Co1—O5 ⁱ	92.42 (16)	C2—C3—C4	119.3 (11)
O1W ⁱ —Co1—O5 ⁱ	94.18 (19)	C2—C3—H3A	120.4

O1W—Co1—O5 ⁱ	85.82 (19)	C4—C3—H3A	120.4
O5—Co1—O5 ⁱ	180.00 (16)	C5—C4—C3	121.5 (11)
O1—P1—O2	116.8 (2)	C5—C4—H4	119.2
O1—P1—O3	112.7 (3)	C3—C4—H4	119.2
O2—P1—O3	107.7 (3)	C4—C5—C6	120.1 (11)
O1—P1—O4	109.8 (2)	C4—C5—H5	119.9
O2—P1—O4	103.4 (3)	C6—C5—H5	119.9
O3—P1—O4	105.4 (3)	C1—C6—C5	120.3 (11)
O5—P2—O7	116.2 (2)	C1—C6—H6A	119.9
O5—P2—O6	112.2 (3)	C5—C6—H6A	119.9
O7—P2—O6	106.4 (3)	N1—C7—C1	114.0 (6)
O5—P2—O4	109.2 (2)	N1—C7—H7A	108.7
O7—P2—O4	109.9 (3)	C1—C7—H7A	108.7
O6—P2—O4	102.0 (3)	N1—C7—H7B	108.7
P1—O1—Co1	134.7 (3)	C1—C7—H7B	108.7
P1—O3—H3	109.5	H7A—C7—H7B	107.6
P2—O4—P1	132.9 (3)	O8—C8—H8A	109.5
P2—O5—Co1	134.7 (2)	O8—C8—H8B	109.5
P2—O6—H6	109.5	H8A—C8—H8B	109.5
Co1—O1W—H1W1	114 (5)	O8—C8—H8C	109.5
Co1—O1W—H2W1	123 (5)	H8A—C8—H8C	109.5
H1W1—O1W—H2W1	114 (3)	H8B—C8—H8C	109.5
C2—O8—C8	117.6 (8)	H1W2—O2W—H2W2	116 (3)
C7—N1—H1A	109.5		
O2—P1—O1—Co1	136.9 (3)	O1W ⁱ —Co1—O5—P2	-116.7 (4)
O3—P1—O1—Co1	-97.5 (4)	O1W—Co1—O5—P2	63.3 (4)
O4—P1—O1—Co1	19.7 (4)	O5 ⁱ —Co1—O5—P2	-67 (100)
O1 ⁱ —Co1—O1—P1	-141 (100)	C8—O8—C2—C3	5.4 (14)
O1W ⁱ —Co1—O1—P1	88.9 (4)	C8—O8—C2—C1	-173.5 (9)
O1W—Co1—O1—P1	-91.1 (4)	C6—C1—C2—O8	-177.8 (8)
O5—Co1—O1—P1	3.2 (4)	C7—C1—C2—O8	4.2 (10)
O5 ⁱ —Co1—O1—P1	-176.8 (4)	C6—C1—C2—C3	3.3 (12)
O5—P2—O4—P1	23.1 (6)	C7—C1—C2—C3	-174.7 (8)
O7—P2—O4—P1	-105.4 (5)	O8—C2—C3—C4	179.9 (9)
O6—P2—O4—P1	142.0 (5)	C1—C2—C3—C4	-1.3 (14)
O1—P1—O4—P2	-39.1 (6)	C2—C3—C4—C5	-0.8 (16)
O2—P1—O4—P2	-164.5 (5)	C3—C4—C5—C6	0.8 (18)
O3—P1—O4—P2	82.6 (5)	C2—C1—C6—C5	-3.3 (14)
O7—P2—O5—Co1	140.4 (4)	C7—C1—C6—C5	174.7 (9)
O6—P2—O5—Co1	-96.9 (4)	C4—C5—C6—C1	1.3 (17)
O4—P2—O5—Co1	15.5 (5)	C6—C1—C7—N1	111.2 (9)
O1 ⁱ —Co1—O5—P2	155.7 (4)	C2—C1—C7—N1	-70.9 (9)
O1—Co1—O5—P2	-24.3 (4)		

Symmetry code: (i) $-x+1, -y+1, -z+1$.

Hydrogen-bond geometry (\AA , $^\circ$)

$D\cdots H\cdots A$	$D\cdots H$	$H\cdots A$	$D\cdots\cdots A$	$D\cdots H\cdots A$
O3—H3 \cdots O2 ⁱⁱ	0.82	1.85	2.553 (6)	143
O6—H6 \cdots O7 ⁱⁱⁱ	0.82	1.77	2.571 (6)	166
O1W—H1W1 \cdots O2 ^{iv}	0.86 (2)	1.98 (3)	2.827 (6)	168 (7)
O1W—H2W1 \cdots O7 ⁱⁱⁱ	0.86 (2)	2.00 (2)	2.851 (6)	171 (8)
N1—H1A \cdots O2W	0.89	1.99	2.840 (8)	159
N1—H1A \cdots O3 ⁱⁱⁱ	0.89	2.53	2.988 (7)	113
N1—H1B \cdots O5 ⁱ	0.89	2.04	2.810 (7)	145
N1—H1C \cdots O1	0.89	2.28	2.944 (7)	131
N1—H1C \cdots O8	0.89	2.42	2.972 (9)	120
O2W—H1W2 \cdots O2 ⁱⁱⁱ	0.85 (2)	2.08 (4)	2.885 (7)	157 (9)
O2W—H2W2 \cdots O7 ^{iv}	0.85 (2)	2.06 (4)	2.876 (7)	161 (9)

Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $x, -y+1/2, z+1/2$; (iii) $x, -y+1/2, z-1/2$; (iv) $-x+1, y+1/2, -z+1/2$.